PHYSICAL REVIEW A VOLUME 27, NUMBER 1 JANUARY 1983

Bounded matrix elements for the quartic-anharmonic oscillator

R. H. Tipping
Physics Department, University of Nebraska at Omaha, Omaha, Nebraska 68182

J. F. Ogilvie
Research School of Chemistry, Australian National University, P. O. Box 4, Canberra ACT 2600, Australia

(Received 18 February 1982)

A method based on quantum-mechanical sum rules is presented in which matrix elements of the displacement and the square of the displacement for a general one-dimensional oscillator are expressed directly in terms of the eigenenergies and the potential parameters. Matrix elements of higher powers of the displacement can then be calculated through an exact hypervirial relation. Two important features of the present method, the rapid convergence and the result that successive approximations are alternately upper and lower bounds to the matrix elements, make the method useful in those cases for which accurate eigenenergies are known. Sample calculations for the quartic-anharmonic oscillator are presented and compared with matrix elements obtained by other iterative schemes.

I. INTRODUCTION

Recently there has been a great deal of interest in the analytical as well as numerical properties of the one-dimensional anharmonic oscillator characterized by the potential[1-10]

$$V(x)=\frac{kx^2}{2}+\lambda x^4 . \tag{1}$$

Bender and Wu[1] have shown that the usual Rayleigh-Schrödinger perturbation series for the ground-state eigenenergy diverges for all $\lambda>0$. Subsequently, several authors have obtained approximate eigenenergies by utilizing alternative convergent summation techniques such as Borel-Padé.[2-4] Various nonperturbative approaches have also been explored. For example, Reid[5] has employed the method of partial fractions, while Biswas *et al.*[6] have assumed a trial wave function of the form

$$\psi(x)=\exp(-x^2/2)\sum_{n=0} C_n x^{2n} , \tag{2}$$

and have solved the resulting Hill determinant numerically for the first few eigenenergies for a range of values of the anharmonic coupling constant λ. In a recent paper, Hioe and Montroll[7] have developed comprehensive analytical approximations using the Bargmann representation.

Other theoretical approaches have also been suggested. For example, several groups have treated the problem through a matrix formalism,[8,9] while Uzes and co-workers[10] have developed iterative techniques in order to compute the eigenenergies.

Paralleling these advances in the determination of accurate eigenenergies, several investigators have developed methods for obtaining progressively better upper and lower bounds for the energy levels. For instance, Bazley and Fox[11] have exploited the variational method, while Reid[12] has used a projection technique due initially to Löwdin.[13]

Most of the work discussed above has been concerned with the general properties and energy levels of the anharmonic oscillator *per se,* although a few authors have discussed possible applications to field theory,[14] and to molecular problems.[15] For these applications, one generally needs matrix elements of various powers of the coordinate x. As is well known, even if approximate eigenfunctions give good eigenenergies, this does not guarantee comparable accuracy when computing matrix elements. To circumvent this difficulty, we shall in the present paper discuss a method for obtaining accurate matrix elements directly from the eigenenergies. The method consists of deriving rapidly convergent expansions for "initial" matrix elements (either $\langle v\,|\,x\,|\,v'\rangle$ or $\langle v\,|\,x^2\,|\,v'\rangle$, depending on whether $v+v'$ is odd or even) by inverting a set of quantum-mechanical sum rules,[16] and then generat-

ing all other matrix elements for the states v,v' through an exact recursion relation obtained from the hypervirial theorem.[17] The theory will be presented in Sec. II for a general one-dimensional potential $V(x)$, and for the specific form given by Eq. (1) in Sec. III.

Furthermore, it has been shown[18] that by taking additional terms in the expansions for the initial elements, one eventually obtains, alternatively, upper and lower bounds to these elements. This information is especially valuable for gauging the absolute accuracy of the matrix elements, and is usually difficult to extract from purely numerical analyses. Finally, in Sec. IV, we will compute numerical results for typical matrix elements which illustrate the convergence and boundedness properties of the method.

II. THEORY

The hypervirial theorem introduced by Hirschfelder[17] expresses a very general quantum-mechanical result: assuming the time-independent Schrödinger equation

$$H\psi_v=\left[-\alpha\frac{d^2}{dx^2}+V(x)\right]\psi_v=E_v\psi_v \tag{3}$$

with $\alpha=\hbar^2/2\mu$, the commutator of the Hamiltonian with an arbitrary time-independent operator W satisfies

$$\langle v'|[H,W]|v\rangle=(E_{v'}-E_v)\langle v'|W|v\rangle\ . \tag{4}$$

For our present purpose it is convenient to choose $W=[H,x^l]$ (where $l=1,2,\ldots$) whence Eq. (4) becomes

$$(E_{v'}-E_v)^2\langle v'|x^l|v\rangle=2\alpha l\left\langle v'\left|x^{l-1}\left[\frac{dV(x)}{dx}\right]\right|v\right\rangle$$
$$+4\alpha l(l-1)\langle v'|x^{l-2}V(x)|v\rangle-2\alpha l(l-1)(E_{v'}+E_v)\langle v'|x^{l-2}|v\rangle$$
$$-\alpha^2 l(l-1)(l-2)(l-3)\langle v'|x^{l-4}|v\rangle\ . \tag{5}$$

This is an exact result. For a polynomial potential, Eq. (5) can be used to generate the matrix elements of higher powers of x from those of lower powers of x if the eigenenergies are known.

Sum rules are likewise quite general quantum-mechanical results which, in contrast to Eq. (5), express relations between diagonal and off-diagonal matrix elements for different states.[16] Briefly, for an Hermitian operator A defined recursively,

$$A_0=A\ ,$$
$$A_a=[H,A_{a-1}]\ , \tag{6}$$

one obtains the well-known results[16]

$$S_v^{2a}\equiv\sum_{v'}(E_{v'}-E_v)^{2a}\langle v|A|v'\rangle\langle v'|A|v\rangle$$
$$=(-1)^a\langle v|(A_a)^2|v\rangle \tag{7a}$$

and

$$S_v^{2a+1}\equiv\sum_{v'}(E_{v'}-E_v)^{2a+1}\langle v|A|v'\rangle\langle v'|A|v\rangle$$
$$=\left[\frac{(-1)^a}{2}\right]\langle v|[A_a,A_{a+1}]|v\rangle\ . \tag{7b}$$

Again, for our present purpose, it is convenient to choose $A_0=x$ or x^2. The results for the first few sum rules for these choices are listed in Tables I and II, where we have introduced the notation $\omega_{v'v}\equiv E_{v'}-E_v$, and the various derivatives of $V(x)$ with respect to x are denoted by primes. Additional sum rules can easily be derived if needed. Note that the first two results (closure and the Thomas-Reiche-Kuhn sum rule) do not depend explicitly on the potential while the remaining results do. In Sec. III we shall illustrate how Eqs. (5) and (7) can be used to determine bounded matrix elements for the quartic-anharmonic oscillator.

III. QUARTIC-ANHARMONIC OSCILLATOR

For the potential given by Eq. (1), Eq. (5) becomes

$$4\alpha\lambda l(l+1)\langle v'|x^{l+2}|v\rangle=[(E_{v'}-E_v)^2-2\alpha kl^2]\langle v'|x^l|v\rangle+2\alpha l(l-1)(E_{v'}+E_v)\langle v'|x^{l-2}|v\rangle$$
$$+\alpha^2 l(l-1)(l-2)(l-3)\langle v'|x^{l-4}|v\rangle\ . \tag{8}$$

TABLE I. General sum rules: $S_v^i(1)\equiv\sum_{v'}\omega_{v'v}^i\,|\,\langle v\,|\,x\,|\,v'\rangle\,|^2$.

i	$S_v^i(1)$
0	$(x^2)_{vv}$
1	α
2	$4\alpha[E_v-(V)_{vv}]$
3	$2\alpha^2(V'')_{vv}$
4	$4\alpha^2(V'^2)_{vv}$
5	$4\alpha^3(V''^2)_{vv}$
6	$8\alpha^3\{[\alpha V''V''''+1.5\alpha(V''')^2+2(E_v-V)(V'')^2]_{vv}\}$
7	$4\alpha^4(\{4V'V''V'''+2(V'')^3+\alpha[(V''')^2-2V'''V''''-2V''V'''']+4(E_v-V)[(V''')^2-2V''V''']\}_{vv})$
8	$16\alpha^4(\{4(E_v-V)^2(V''')^2+2(E_v-V)[2\alpha(V'''')^2-\alpha V'''V''''-2V'V''V''']$ $+\alpha^2[0.25(V'''')^2-V''''V''''''-(V''')^2]$ $-\alpha[V'V''V''''+4V'V'''V''''+2(V'')^2V''''']+(V'V'')^2\}_{vv})$

Inspection of this equation reveals that for a given v and v', only one initial element and the eigenenergies are needed in order to generate all other matrix elements of higher powers of x. To obtain this initial element, consider the sum rules discussed above. Using the results listed in Tables I and II and Eq. (8), the first few sum rules for the quartic-anharmonic oscillator are listed in Tables III and IV, where we have introduced the notation $\langle v'\,|\,x^l\,|\,v\rangle\equiv(x^l)_{v'v}$. These reduce to the well-known harmonic oscillator (HO) results in the limit $\lambda\to 0$; i.e.,

$$S_v^i(1)^{\rm HO}=2\alpha\left[\hbar\left[\frac{k}{\mu}\right]^{1/2}\right]^{i-1}\left[\left[\frac{1+(-1)^i}{2}\right]v+\tfrac{1}{2}\right] \tag{9}$$

and

$$S_v^i(2)^{\rm HO}=\frac{2^{i-1}\alpha\hbar^i}{k}\left[\frac{k}{\mu}\right]^{i/2}\{[1+(-1)^i]v^2+[3-(-1)^i]v+2\}$$

TABLE II. General sum rules: $S_v^i(2)\equiv\sum_{v'\neq v}\omega_{v'v}^i\,|\,\langle v\,|\,x^2\,|\,v'\rangle\,|^2$.

i	$S_v^i(2)$
0	$(x^4)_{vv}-(x^2)_{vv}^2$
1	$4\alpha(x^2)_{vv}$
2	$12\alpha^2+16\alpha[x^2(E_v-V)]_{vv}$
3	$8\alpha^2\{[x^2V''+xV'+4(E_v-V)]_{vv}\}$
4	$16\alpha^2\{[4(E_v-V)^2-4xV'(E_v-V)+x^2(V')^2]_{vv}\}$
5	$16\alpha^3\{[(xV''+3V')^2]_{vv}\}$
6	$96\alpha^3(\{(E_v-V)[6(V')^2+4xV'V''+\frac{2}{3}(xV'')^2]$ $+\alpha[5V'V'''+8(V'')^2+xV'V''''+\frac{17}{3}xV''V'''$ $+0.5(xV''')^2+\frac{1}{3}x^2V''V'''']\}_{vv})$
7	$16\alpha^4(\{8(E_v-V)[(xV'''+4V'')^2-0.5(xV''+3V')(xV''''+5V''')]$ $+\alpha[(2xV''''+10V''')^2+2(xV'''+4V'')(xV''''+6V'''')$ $-(xV''+3V')(xV''''''+7V'''')]$ $+2(xV''+3V')[xV'V'''+x(V'')^2+7V'V'']\}_{vv})$
8	$64\alpha^4[((E_v-V)^2(2xV'''+8V'')^2-4(E_v-V)(xV'''+4V'')[xV'V''+3(V')^2]+[xV'V''+3(V')^2]^2$ $-\alpha\{6(E_v-V)(xV'''+4V'')(xV''''+6V'''')+2[x(V'')^2+3V'V''](xV''''+5V''')$ $+2(xV'V'''+4V'V'')(xV''''+5V''')+[xV'V''+3(V')^2](xV''''+6V'''')\}$ $-\alpha^2[\frac{11}{4}(xV''''+6V'''')^2+5(xV''''+5V''')(xV''''''+7V'''')$ $+2(xV'''+4V'')(xV''''''+8V'''''')]_{vv}]$

TABLE III. Quartic-anharmonic oscillator sum rules: $S_v^i(1) \equiv \sum_{v'} \omega_{v'v}^i \, | \langle v \, | \, x \, | \, v' \rangle \, |^2$.

i	$S_v^i(1)$
0	$(x^2)_{vv}$
1	α
2	$\frac{8}{3}\alpha E_v - \frac{2}{3}\alpha k (x^2)_{vv}$
3	$2\alpha^2[k + 12\lambda (x^2)_{vv}]$
4	$\frac{4}{15}\alpha^2[8E_v k + 72\alpha\lambda + (144E_v\lambda + 7k^2)(x^2)_{vv}]$
5	$4\alpha^3[48E_v\lambda + k^2 - 24k\lambda (x^2)_{vv}]$
6	$\frac{8}{7}\alpha^3[(192E_v^2\lambda + \frac{52}{3}E_v k^2 + 24\alpha k\lambda) + (-144E_v k\lambda + 3744\alpha\lambda^2 - \frac{31}{3}k^3)(x^2)_{vv}]$
7	$\frac{8}{5}\alpha^4[(-1008E_v k\lambda + 7488\alpha\lambda^2 + 5k^3) + 108\lambda(112E_v\lambda + 11k^2)(x^2)_{vv}]$
8	$\frac{16}{15}\alpha^4[(-2304E_v^2 k\lambda + 201\,984E_v\alpha\lambda^2 - 112E_v k^3 + 432\alpha k^2\lambda) + (16\,128E_v^2\lambda^2 + 3168E_v k^2\lambda - 13\,056\alpha k\lambda^2 + 127k^4)(x^2)_{vv}]$

when we make the obvious identification

$$\lim_{\lambda\to 0}\frac{1}{3\lambda}(E_v - k\langle v \, | \, x^2 \, | \, v\rangle) \Longrightarrow \langle v \, | \, x^4 \, | \, v\rangle^{\mathrm{HO}} = \frac{3\alpha}{k}(v^2 + v + \tfrac{1}{2}) , \tag{10}$$

and to the quartic oscillator results[18] in the limit of $k \to 0$. [There are two misprints in Table I of Ref. 18: the coefficient of E_v^2 in $S_v^6(1)$ should read $2/a$, and the multiplicative factor for $S_v^8(2)$ should be 36 864/55.]

To illustrate the use of the anharmonic oscillator sum rules, consider the specific example: $l = 1$ and v is even. This will enable us to find the matrix elements for all powers of x between states for which $v + v'$ is odd. With this choice, the sum rules can be written in matrix form

$$\begin{pmatrix} 1 & 1 & 1 & \cdots \\ \omega_{1v} & \omega_{3v} & \omega_{5v} & \cdots \\ \omega_{1v}^2 & \omega_{3v}^2 & \omega_{5v}^2 & \cdots \\ . & . & . & \\ . & . & . & \\ . & . & . & \end{pmatrix} \begin{pmatrix} x_{v1}^2 \\ x_{v3}^2 \\ x_{v5}^2 \\ . \\ . \\ . \end{pmatrix} = \begin{pmatrix} S_v^0(1) \\ S_v^1(1) \\ S_v^2(1) \\ . \\ . \\ . \end{pmatrix} , \tag{11}$$

TABLE IV. Quartic-anharmonic oscillator sum rules: $S_v^i(2) \equiv \sum_{v' \neq v} \omega_{v'v}^i \, | \langle v \, | \, x^2 \, | \, v' \rangle \, |^2$.

i	$S_v^i(2)$
0	$\frac{1}{3\lambda}[E_v - k(x^2)_{vv}] - (x^2)_{vv}^2$
1	$4\alpha(x^2)_{vv}$
2	$\frac{4}{15}\alpha\left[\frac{-2E_v k}{\lambda} + 27\alpha + \left[24E_v + \frac{2k^2}{\lambda}\right](x^2)_{vv}\right]$
3	$32\alpha^2[2E_v - k(x^2)_{vv}]$
4	$\frac{64}{7}\alpha^2\left[8E_v^2 + \frac{E_v k^2}{3\lambda} + (4.5\alpha k) + \left[-6E_v k + 135\alpha\lambda - \frac{k^3}{3\lambda}\right](x^2)_{vv}\right]$
5	$\frac{256}{5}\alpha^3[(-4E_v k + 54\alpha\lambda) + (108E_v\lambda + 9k^2)(x^2)_{vv}]$
6	$\frac{512}{15}\alpha^3\left[\left[-12E_v^2 k + 1482E_v\alpha\lambda - \frac{E_v k^3}{\lambda} + \frac{27\alpha k^2}{2}\right] + \left[144E_v^2\lambda + 24E_v k^2 - 960\alpha k\lambda + \frac{k^4}{\lambda}\right](x^2)_{vv}\right]$
7	$2048\alpha^4[72E_v^2\lambda + (6E_v k^2) + (-72E_v k\lambda + 810\alpha\lambda^2 - 5k^3)(x^2)_{vv}]$
8	$\frac{4096}{11}\alpha^4\left[\left[288E_v^3\lambda + 48E_v^2 k^2 + \frac{5E_v k^4}{3\lambda} - \frac{18\,726E_v\alpha k\lambda}{5} + \frac{90\,801\alpha^2\lambda^2}{5} + 4.5\alpha k^3\right] + \left[-360E_v^2 k\lambda + \frac{185\,652E_v\alpha\lambda^2}{5} - 50E_v k^3 + \frac{21\,471\alpha k^2\lambda}{5} - \frac{5k^5}{3\lambda}\right](x^2)_{vv}\right]$

where all odd matrix elements vanish from parity. Assuming that the $S_v^i(1)$ are known [actually, the matrix element x_{vv}^2 appearing in $S_v^i(1)$ is not known, but can be treated as one of the unknowns in the infinite set of equations without affecting the conclusions of the discussion below[18]] and finite, Eq. (11) implies that the squares of the matrix elements must approach zero faster than any power n of the energy differences; i.e.,

$$\lim_{v'\to\infty}(\omega_{v'v})^n\langle v'\mid x\mid v\rangle^2\to 0\ . \tag{12}$$

Thus, one can truncate the infinite set of equations and obtain the nth approximation to the first n matrix elements

$$\begin{bmatrix} x_{v1}^2 \\ x_{v3}^2 \\ \cdot \\ \cdot \\ \cdot \\ x_{v2n-1}^2 \end{bmatrix} = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ \omega_{1v} & \omega_{3v} & & \omega_{2n-1v} \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \omega_{1v}^{n-1} & & & \omega_{2n-1v}^{n-1} \end{bmatrix}^{-1} \begin{bmatrix} S_v^0(1) \\ S_v^1(1) \\ \cdot \\ \cdot \\ \cdot \\ S_v^{n-1}(1) \end{bmatrix} . \tag{13}$$

In theory, a sufficiently large n can be chosen so that any desired accuracy can be obtained (provided, of course, that the eigenenergies are also known with adequate precision so that round-off errors do not become important). In practice, however, usually only a few terms are required to yield reasonably accurate matrix elements because of the rapid convergence of successive approximations. In fact, for the harmonic oscillator, Eq. (13) gives the exact results at each level of approximation. One would thus expect rapid convergence for small λ (see below), and indeed the convergence is quite rapid for the pure quartic oscillator.[18]

The formal solution to Eq. (13) can be written since the matrix of eigenenergy differences is of the form known as an "alternate" matrix and has a well-known inverse.[19] Each element of a given row of the inverse matrix is a quotient, the denominator of which is a product of the ordered differences between the eigenvalues, while the numerators are the "simple symmetric functions" formed from the eigenenergy differences with one omitted. Specifically, we can write for the nth approximation

$$x_{vj}^2=\frac{1}{\prod_{l=1}^{n}{}'\,\omega_{2l-1,j}}\sum_{i=0}^{n-1}C_iS_v^i(1)\ , \tag{14}$$

where C_i is the coefficient of the t^{n-i-1} term of the function

$$\prod_{l=1}^{n}{}'(\omega_{2l-1,v}t-1)\ . \tag{15}$$

The prime on the product notation indicates that the term $l=(j+1)/2$ is to be omitted. While these formulas are convenient for numerical programming, they do not shed any light on the boundedness of the successive approximations. As discussed elsehwere,[18] this can be shown to follow from the Schweinsian expansion[19] of the formal solution through Cramer's rule.[18] This will be illustrated in Sec. IV, where we calculate numerical results.

IV. QUARTIC-ANHARMONIC MATRIX ELEMENTS: NUMERICAL RESULTS

In order to illustrate the method described above for the calculation of initial matrix elements, and to

TABLE V. Successive approximations to the initial quartic-anharmonic matrix elements using the sum rules from Table III and comparison with results from other methods.

n	$(x^2)_{00}$	$(x)_{01}^2$	$(x)_{03}^2\times 10^3$	$(x)_{05}^2\times 10^6$
2	0.355 862	0.355 862		
3	0.354 838	0.354 430	0.407 465	
4	0.354 840	0.354 434	0.405 379	0.508 948
5	0.354 840	0.354 434	0.405 387	0.505 371
6	0.354 840	0.354 434	0.405 387	0.505 371
Ref. 9		0.354 434	0.405 387	0.505 421
Ref. 10		0.354 437	0.405 080	0.435 204

facilitate the comparison with other published results,[9,10] we will consider the particular case $\alpha=\frac{1}{2}$, $k=1$, and $\lambda=\frac{1}{4}$. The Hamiltonian is thus given by

$$H=-\frac{1}{2}\frac{d^2}{dx^2}+\frac{1}{2}x^2+\frac{1}{4}x^4\,, \tag{16}$$

and for the calculation we will assume the eigenenergies published by Li *et al.*[9] We will only consider the case where $v=0$ explicitly, since the other vibrational levels can be treated in an identical way.

With the use of Eq. (13) and the sum rules given in Table III, the successive approximations to the matrix elements $(x^2)_{00}$ and $(x_{0j})^2$ for odd j are obtained by increasing the number of simultaneous equations n. These results are presented in Table V along with the results obtained by other workers using different methods. Analogous reuslts for $(x^2)^2_{0j}$ for even j, obtained through the sum rules in Table IV, are displayed in Table VI.

Both the rapid convergence and boundedness of the successive approximations are apparent from these numerical results. The converged results are in excellent agreement with those of Li *et al.*,[9] but agree less well with those computed by Uzes and co-workers[10] by a different iterative scheme. In the present method, the factor which limits the accuracy of the matrix elements is the accuracy of the corresponding energy eigenvalues.

Initial matrix elements for other choices of α, k, and λ can be obtained in the same way. In particular, it should be noted that in the case for which $k<0$ the potential is a double minimum well[20] with a barrier height of $k^2/16\lambda$. The above results are applicable in this case provided one uses the energies as measured from the bottom of the well.

TABLE VI. Successive approximations to the initial quartic-anharmonic matrix elements using the sum rules from Table IV.

n	$(x)^2_{02}$	$(x)^2_{04}\times 10^2$	$(x)^2_{06}\times 10^5$
2	0.227 495	0.137 608	
3	0.227 500	0.136 589	0.477 154
4	0.227 500	0.136 594	0.472 472

Finally, we wish to reiterate that matrix elements of higher powers of x can be generated from the initial elements through the exact hypervirial relation [Eq. (5)]. The use of sum rules, in contradistinction to asymptotic solutions of the system of Eqs. (5),[21] provides a very simple and rapidly convergent algorithm for the calculations of bounded matrix elements provided that the corresponding eigenenergies are known.

ACKNOWLEDGMENT

One of the authors (R.H.T.) would like to acknowledge partial financial support from the Committee on Research, University of Nebraska at Omaha.

[1]C. Bender and T. T. Wu, Phys. Rev. Lett. 21, 406 (1968); Phys. Rev. 184, 1231 (1969).
[2]B. Simon, Ann. Phys. (N.Y.) 58, 76 (1970).
[3]J. Loeffel, A. Martin, B. Simon, and A. Wightman, Phys. Lett. 30B, 656 (1969).
[4]S. Graffi, V. Grecchi, and B. Simon, Phys. Lett. 32B, 631 (1970); S. Graffi, V. Grecchi, and G. Turchetti, Nuovo Cimento 43, 313 (1970); S. Graffi, J. Math. Phys. 19, 1002 (1978).
[5]C. Reid, Int. J. Quant. Chem. 1, 521 (1967).
[6]S. N. Biswas, K. Datta, R. P. Saxena, P. K. Srivastava, and V. S. Varma, J. Math. Phys. 14, 1190 (1973).
[7]F. T. Hioe and E. W. Montroll, J. Math. Phys. 16, 1945 (1975).
[8]F. R. Halpern, J. Math. Phys. 14, 219 (1973); F. R. Halpern and T. W. Yonkman, J. Math. Phys. 15, 1718 (1974).
[9]C.-T. Li, A. Klein, and F. Krejs, Phys. Rev. D 12, 2311 (1975).
[10]J. H. Henkel and C. A. Uzes, Phys. Rev. D 8, 4430 (1973); C. A. Uzes, *ibid.* 14, 3362 (1976).
[11]N. Bazley and D. Fox, Phys. Rev. 124, 483 (1961).
[12]C. Reid, J. Chem. Phys. 43, S186 (1965).
[13]P.-O. Löwdin, J. Chem. Phys. 43, S175 (1965).
[14]L. I. Schiff, Phys. Rev. 92, 766 (1953).
[15]S. I. Chan, D. Stelman, and L. E. Thompson, J. Chem. Phys. 41, 2828 (1964).
[16]R. Jackiw, Phys. Rev. 157, 1220 (1967).
[17]J. O. Hirschfelder, J. Chem. Phys. 33, 1462 (1960); R. H. Tipping, *ibid.* 59, 6433 (1973); 59, 6443 (1973).
[18]R. H. Tipping, J. Mol. Spectrosc. 59, 8 (1976); 73, 400 (1978).
[19]A. C. Aitken, *Determinants and Matrices* (Oliver and Boyd, Edinburgh, 1956).
[20]J. Laane, Appl. Spectrosc. 24, 73 (1970).
[21]J. L. Richardson and R. Blankenbecler, Phys. Rev. D 19, 496 (1979).